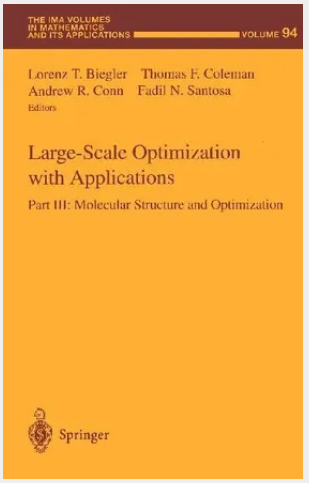
Biegler / Coleman / Conn

Large-Scale Optimization with Applications

Part III: Molecular Structure and Optimization

Many important molecular conformation problems, such as protein folding, are expressed as global minimization problems. It is the fact that local minimization is insufficient, that markedly differentiates this volume from the previous two. Unfortunately, global minimization problems that result from models of molecular conformation are usually intractable. For example, simple 1-dimensional versions of distance conformation problems are NP-hard. Nevertheless, there has been significant recent progress in the design of promising heuristic strategies (often involving the use of high- performance parallel computers) for computing approximate global minimizers. The purpose of the sessions represented in this volume was to discuss the new algorithmic advances for global minimization in the context of protein folding and related molecular minimization problems. Emphasis was on practical shortcomings of current approaches, outstanding problems and questions, and the use of high-performance parallel computers.

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